Lanthanum ruthenium indide, La(21)Ru(9+x)In(5-x) (x = 1.2).

Anna I. Tursina, Sergei G. Cherviakov, Henri Noël, Vladimir V. Chernyshev, Yuri D. Seropegin

Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Lanthanum ruthenium indide, $La_{21}Ru_{9+x}In_{5-x}$ (x = 1.2)

Anna I. Tursina,[a] Sergei G. Cherviakov,[a] Henri Noël,[b] Vladimir V. Chernyshev[a]* and Yuri D. Seropegin[a]

[a]Department of Chemistry, Moscow State University, Leninskie Gory 1/3, 119 992 Moscow, Russian Federation, and [b]Laboratoire de Chimie du Solide et Matériaux, UMR6226 CNRS-Université de Rennes 1, Avenue du Général Leclerc, 30542 Rennes, France
Correspondence e-mail: vladimir@struct.chem.msu.ru

Received 26 March 2010; accepted 20 April 2010

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(La–Ru) = 0.001 Å; disorder in main residue; R factor = 0.036; wR factor = 0.062; data-to-parameter ratio = 22.7.

$La_{21}Ru_{9+x}In_{5-x}$ (Pearson symbol *tI*140) is isotypic to the filled Y_3Rh_2-type structure, from which it can be derived through an ordered substitution at two sites. One of the square-prismatic sites (site symmetry ..*m*) is occupied by a mixture of Ru and In atoms and one of the square-antiprismatic sites (4/*m*..) is fully occupied by In atoms.

Related literature

For related structures, see: Zaremba *et al.* (2007); Moreau *et al.* (1976). For standardization of crystal structures, see: Gelato & Parthé (1987).

Experimental

Crystal data

$La_{21}Ru_{10.16}In_{3.84}$
M_r = 4384.89
Tetragonal, $I4/mcm$
a = 12.1298 (3) Å
c = 25.9820 (7) Å
V = 3822.79 (17) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 28.98 mm^{-1}
T = 293 K
0.06 × 0.05 × 0.05 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: for a sphere (*WinGX*; Farrugia, 1999)
T_{min} = 0.243, T_{max} = 0.261
22423 measured reflections
1202 independent reflections
927 reflections with $I > 2\sigma(I)$
R_{int} = 0.087

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.062
S = 1.12
1202 reflections
53 parameters
$\Delta\rho_{max}$ = 2.00 e Å^{-3}
$\Delta\rho_{min}$ = −2.74 e Å^{-3}

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXL97*.

This work was supported by the RFBR project 080300702*a*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: MG2098).

References

Brandenburg, K. (1999). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Gelato, L. M. & Parthé, E. (1987). *J. Appl. Cryst.* **20**, 139–143.
Moreau, J.-M., Paccard, D. & Parthé, E. (1976). *Acta Cryst.* B**32**, 1767–1771.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zaremba, R., Rodewald, U. Ch., Zaremba, V. I. & Pöttgen, R. (2007). *Z. Naturforsch. Teil B*, **62**, 1397–1406.

supplementary materials

Acta Cryst. (2010). E**66**, i40 [**doi:10.1107/S1600536810014509**]

Lanthanum ruthenium indide, $La_{21}Ru_{9+x}In_{5-x}$ (x = 1.2)

A. I. Tursina, S. G. Cherviakov, H. Noël, V. V. Chernyshev and Y. D. Seropegin

Comment

New rare-earth metal-rich indium compounds $RE_3T_{2-x}In_x$ (RE = Gd, Tb, Dy, Ho, Er, Tm; T = Rh, Pd, Ir) have been recently synthesized (Zaremba et al., 2007). They can be regarded as extensions of the parent binaries RE_3T_2 with either the Y_3Rh_2- (T = Rh, Ir) or U_3Si_2-type (T = Pd) structures into the ternary RE–T–In systems. In contrast, $La_{21}Ru_{9+x}In_{5-x}$, presented here, is strictly a ternary compound with no corresponding La-Ru binary of the same stoichiometry.

In the Y_3Rh_2–type structure, six crystallographically independent transition metal sites are available with trigonal prismatic, square prismatic, and square antiprismatic coordination environments (Moreau et al., 1976). The structure of $La_{21}Ru_{9+x}In_{5-x}$ is derived through an ordered substitution at two sites, with the square prismatic site (16l) occupied by a mixture of Ru and In atoms and one of the square antiprismatic sites (4c) occupied fully by In atoms (Fig. 1). This suggests the existence of a solid solution, as confirmed by EDX measurements which revealed a homogeneity range of ca. 3 at.% in $La_{21}Ru_{9+x}In_{5-x}$.

Experimental

The title compound was prepared by arc-melting of the constituent elements (La, 99.8%; Ru, 99.9%, In, 99.999%) under a high purity argon atmosphere on a water-cooled cooper hearth. The arc-melted button, with nominal composition $La_{59.26}Ru_{29.63}In_{11.11}$, was turned over and remelted to ensure its homogeneity. The weight loss was less than 1%. The sample was annealed in an evacuated quartz ampoule at 870 K for 600 h and quenched in cold water. The single crystal was selected from the crushed sample.

EDX analysis of the majority phase in a number of samples revealed that the composition of the new compound ranges from $La_{58.8}Ru_{26.2}In_{15.0}$ to $La_{61.1}Ru_{28.3}In_{10.7}$ with an uncertainty of about 1 at.% for each element. Thus the homogeneity range of the title compound is approximately 3 at.% at 870 K.

Refinement

The atomic parameters were standardized with the program STRUCTURE TIDY (Gelato & Parthé, 1987). The highest peak and the deepest hole in the final difference map are located 0.69 Å from La2 and 0.82 Å, respectively, from Ru1.

Figures

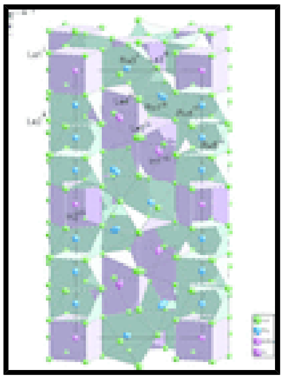


Fig. 1. Structure of the title compound emphasizing the coordination polyhedra, with atom labelling shown and displacement ellipsoids drawn at the 50% probability level.

lanthanum ruthenium indium (21/10.2/3.8)

Crystal data

$La_{21}Ru_{10.16}In_{3.84}$	$D_x = 7.619$ Mg m^{-3}
$M_r = 4384.89$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Tetragonal, $I4/mcm$	Cell parameters from 12585 reflections
Hall symbol: -I 4 2c	$\theta = 2.9$–27.5°
$a = 12.1298$ (3) Å	$\mu = 28.98$ mm^{-1}
$c = 25.9820$ (7) Å	$T = 293$ K
$V = 3822.79$ (17) Å^3	Prism, metallic-dark-grey
$Z = 4$	0.06 × 0.05 × 0.05 mm
$F(000) = 7329$	

Data collection

Nonius KappaCCD diffractometer	1202 independent reflections
Radiation source: fine-focus sealed tube	927 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.087$
φ and ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 3.7°$
Absorption correction: for a sphere (WinGX; Farrugia, 1999)	$h = -15 \rightarrow 15$
$T_{min} = 0.243$, $T_{max} = 0.261$	$k = -15 \rightarrow 15$
22423 measured reflections	$l = -33 \rightarrow 32$

Refinement

Refinement on F^2	0 restraints
Least-squares matrix: full	Primary atom site location: structure-invariant direct methods
$R[F^2 > 2\sigma(F^2)] = 0.036$	Secondary atom site location: difference Fourier map
$wR(F^2) = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.0131P)^2 + 224.3566P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} < 0.001$
1202 reflections	$\Delta\rho_{max} = 2.00$ e Å^{-3}
53 parameters	$\Delta\rho_{min} = -2.74$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
La1	0.07818 (5)	0.20842 (5)	0.07297 (2)	0.01886 (15)	
La2	0.20391 (6)	0.07950 (6)	0.19170 (2)	0.02653 (17)	
La3	0.85106 (8)	0.35106 (8)	0.0000	0.0208 (3)	
La4	0.0000	0.5000	0.10584 (5)	0.0255 (3)	
La5	0.0000	0.5000	0.2500	0.0615 (8)	
Ru1	0.81308 (11)	0.31308 (11)	0.10986 (6)	0.0429 (4)	
Ru2	0.65628 (8)	0.15628 (8)	0.18661 (5)	0.0287 (4)	0.29 (4)
Ru3	0.59671 (12)	0.09671 (12)	0.0000	0.0247 (4)	
Ru4	0.0000	0.0000	0.12798 (6)	0.0207 (4)	
Ru5	0.0000	0.0000	0.2500	0.0213 (5)	
In1	0.65628 (8)	0.15628 (8)	0.18661 (5)	0.0287 (4)	0.71 (4)
In2	0.0000	0.0000	0.0000	0.0200 (5)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
La1	0.0226 (3)	0.0185 (3)	0.0154 (3)	−0.0006 (3)	0.0001 (2)	0.0002 (2)
La2	0.0305 (4)	0.0311 (4)	0.0180 (3)	−0.0036 (3)	0.0003 (3)	−0.0001 (3)
La3	0.0218 (4)	0.0218 (4)	0.0188 (6)	0.0021 (6)	0.000	0.000
La4	0.0260 (4)	0.0260 (4)	0.0247 (7)	0.0035 (6)	0.000	0.000
La5	0.0793 (13)	0.0793 (13)	0.0258 (12)	0.000	0.000	0.000
Ru1	0.0471 (6)	0.0471 (6)	0.0345 (8)	0.0213 (8)	−0.0168 (6)	−0.0168 (6)
Ru2	0.0244 (5)	0.0244 (5)	0.0372 (8)	0.0073 (5)	−0.0070 (4)	−0.0070 (4)
Ru3	0.0270 (6)	0.0270 (6)	0.0202 (9)	0.0055 (8)	0.000	0.000
Ru4	0.0195 (5)	0.0195 (5)	0.0232 (9)	0.000	0.000	0.000
Ru5	0.0199 (8)	0.0199 (8)	0.0241 (12)	0.000	0.000	0.000
In1	0.0244 (5)	0.0244 (5)	0.0372 (8)	0.0073 (5)	−0.0070 (4)	−0.0070 (4)
In2	0.0206 (7)	0.0206 (7)	0.0190 (10)	0.000	0.000	0.000

Geometric parameters (Å, °)

La1—Ru1^{i}	3.0174 (15)	La4—La2^{i}	4.3365 (10)
La1—Ru3^{ii}	3.0385 (12)	La5—In1^{xxix}	3.1464 (14)
La1—Ru4	3.0550 (10)	La5—Ru2^{xxix}	3.1464 (14)
La1—In2	3.2992 (6)	La5—In1^{xii}	3.1464 (14)
La1—In1^{i}	3.5084 (13)	La5—Ru2^{xii}	3.1464 (14)
La1—Ru2^{i}	3.5084 (13)	La5—In1^{i}	3.1464 (14)
La1—Ru1^{iii}	3.5875 (11)	La5—In1^{xxv}	3.1464 (14)
La1—La2^{iv}	3.6299 (9)	La5—Ru2^{i}	3.1464 (14)
La1—La1^{v}	3.6607 (13)	La5—Ru2^{xxv}	3.1464 (14)
La1—La4	3.7600 (7)	La5—La4^{xxx}	3.7457 (13)
La1—La3^{iii}	3.7653 (7)	La5—La2^{i}	4.0154 (7)
La1—La2	3.7798 (9)	La5—La2^{iv}	4.0154 (7)
La1—La1^{vi}	3.7919 (11)	La5—La2^{xxxi}	4.0154 (7)
La1—La1^{iv}	3.8185 (9)	La5—La2^{xii}	4.0154 (7)
La1—La1^{vii}	3.8185 (9)	La5—La2^{xxviii}	4.0154 (7)
La1—La3^{ii}	3.8822 (12)	La5—La2^{xxv}	4.0154 (7)
La2—Ru1^{i}	2.8235 (14)	La5—La2^{xxix}	4.0154 (7)
La2—Ru5	3.0565 (7)	La5—La2^{x}	4.0154 (7)
La2—Ru4	3.1286 (11)	Ru1—La2^{xxiii}	2.8235 (14)
La2—In1^{i}	3.2592 (13)	Ru1—La2^{xxii}	2.8235 (14)
La2—Ru2^{i}	3.2592 (13)	Ru1—La1^{xxii}	3.0174 (15)
La2—In1^{viii}	3.3276 (8)	Ru1—La1^{xxiii}	3.0174 (15)
La2—Ru2^{viii}	3.3276 (8)	Ru1—La4^{xvi}	3.2082 (19)
La2—La2^{ix}	3.5915 (13)	Ru1—La1^{xvi}	3.5875 (11)
La2—La1^{vii}	3.6299 (9)	Ru1—La1^{xx}	3.5875 (11)
La2—La2^{x}	3.7060 (13)	Ru2—La5^{xii}	3.1464 (14)
La2—In1^{xi}	3.7068 (12)	Ru2—La2^{xxii}	3.2592 (13)
La2—Ru2^{xi}	3.7068 (12)	Ru2—La2^{xxiii}	3.2592 (13)
La2—La2^{v}	3.7154 (14)	Ru2—La2^{v}	3.3276 (8)
La2—La2^{vii}	3.7544 (10)	Ru2—La2^{viii}	3.3276 (8)
La2—La2^{iv}	3.7544 (10)	Ru2—La4^{xiii}	3.4047 (15)
La2—La5^{xii}	4.0154 (7)	Ru2—La1^{xxii}	3.5084 (13)
La2—La4^{xiii}	4.3365 (10)	Ru2—La1^{xxiii}	3.5084 (13)
La3—Ru1^{vi}	2.9278 (17)	Ru2—La2^{xxxii}	3.7068 (12)
La3—Ru1	2.9278 (17)	Ru2—La2^{xi}	3.7068 (12)
La3—Ru3^{xiv}	3.0463 (16)	Ru3—La1^{xiv}	3.0385 (12)
La3—Ru3^{xv}	3.0463 (16)	Ru3—La1^{xxii}	3.0385 (12)
La3—La4^{xvi}	3.7536 (13)	Ru3—La1^{xxiii}	3.0385 (12)

La3—La4^{xvii}	3.7536 (13)	Ru3—La1^{xxi}	3.0385 (12)
La3—La1^{xvi}	3.7653 (7)	Ru3—La3^{ii}	3.0463 (16)
La3—La1^{xviii}	3.7653 (7)	Ru3—La3^{xxxiii}	3.0463 (16)
La3—La1^{xix}	3.7653 (7)	Ru3—La4^{xiv}	3.2115 (15)
La3—La1^{xx}	3.7653 (7)	Ru3—La4^{xiii}	3.2115 (15)
La3—La1^{xiv}	3.8822 (12)	Ru4—La1^{xxxiv}	3.0550 (10)
La3—La1^{xxi}	3.8822 (12)	Ru4—La1^{iv}	3.0550 (10)
La3—La1^{xxii}	3.8822 (12)	Ru4—La1^{vii}	3.0550 (10)
La3—La1^{xxiii}	3.8822 (12)	Ru4—La2^{iv}	3.1286 (11)
La4—Ru1^{xxiv}	3.2082 (19)	Ru4—La2^{xxxiv}	3.1286 (11)
La4—Ru1^{iii}	3.2082 (19)	Ru4—La2^{vii}	3.1286 (11)
La4—Ru3^{xxv}	3.2115 (15)	Ru5—La2^{x}	3.0565 (7)
La4—Ru3^{ii}	3.2115 (15)	Ru5—La2^{xxxiv}	3.0565 (7)
La4—In1^{i}	3.4047 (15)	Ru5—La2^{vii}	3.0565 (7)
La4—In1^{xxv}	3.4047 (15)	Ru5—La2^{ix}	3.0565 (7)
La4—Ru2^{i}	3.4047 (15)	Ru5—La2^{xxxv}	3.0565 (7)
La4—Ru2^{xxv}	3.4047 (15)	Ru5—La2^{xxxvi}	3.0565 (7)
La4—La5	3.7457 (13)	Ru5—La2^{iv}	3.0565 (7)
La4—La3^{iii}	3.7536 (13)	In2—La1^{xxxvii}	3.2992 (6)
La4—La3^{xvii}	3.7536 (13)	In2—La1^{iv}	3.2992 (6)
La4—La1^{v}	3.7600 (7)	In2—La1^{xxxiv}	3.2992 (6)
La4—La1^{xxvi}	3.7600 (7)	In2—La1^{vii}	3.2992 (6)
La4—La1^{xxvii}	3.7600 (7)	In2—La1^{xxxviii}	3.2992 (6)
La4—La2^{xxviii}	4.3365 (10)	In2—La1^{vi}	3.2992 (6)
La4—La2^{xxv}	4.3365 (10)	In2—La1^{xxxix}	3.2992 (6)
La4—La2^{iv}	4.3365 (10)		

Ru1^{i}—La1—Ru3^{ii}	101.28 (4)	Ru2^{xxv}—La4—La1^{v}	143.53 (3)
Ru1^{i}—La1—Ru4	94.19 (3)	La5—La4—La1^{v}	103.13 (2)
Ru3^{ii}—La1—Ru4	163.46 (3)	La3^{iii}—La4—La1^{v}	99.50 (3)
Ru1^{i}—La1—In2	112.81 (4)	La3^{xvii}—La4—La1^{v}	60.151 (15)
Ru3^{ii}—La1—In2	104.998 (19)	La1—La4—La1^{v}	58.26 (2)
Ru4—La1—In2	62.97 (3)	Ru1^{xxiv}—La4—La1^{xxvi}	119.600 (14)
Ru1^{i}—La1—In1^{i}	61.19 (4)	Ru1^{iii}—La4—La1^{xxvi}	61.370 (13)
Ru3^{ii}—La1—In1^{i}	98.12 (2)	Ru3^{xxv}—La4—La1^{xxvi}	50.94 (3)
Ru4—La1—In1^{i}	94.43 (3)	Ru3^{ii}—La4—La1^{xxvi}	103.96 (4)
In2—La1—In1^{i}	156.88 (2)	In1^{i}—La4—La1^{xxvi}	143.53 (3)
Ru1^{i}—La1—Ru2^{i}	61.19 (4)	In1^{xxv}—La4—La1^{xxvi}	58.39 (2)
Ru3^{ii}—La1—Ru2^{i}	98.12 (2)	Ru2^{i}—La4—La1^{xxvi}	143.53 (3)
Ru4—La1—Ru2^{i}	94.43 (3)	Ru2^{xxv}—La4—La1^{xxvi}	58.39 (2)
In2—La1—Ru2^{i}	156.88 (2)	La5—La4—La1^{xxvi}	103.13 (2)

In1^{i}—La1—Ru2^{i}	0.00 (2)	La3^{iii}—La4—La1^{xxvi}	60.151 (15)
Ru1^{i}—La1—Ru1^{iii}	142.38 (5)	La3^{xvii}—La4—La1^{xxvi}	99.50 (3)
Ru3^{ii}—La1—Ru1^{iii}	87.58 (5)	La1—La4—La1^{xxvi}	115.02 (2)
Ru4—La1—Ru1^{iii}	83.66 (3)	La1^{v}—La4—La1^{xxvi}	153.75 (4)
In2—La1—Ru1^{iii}	99.62 (3)	Ru1^{xxiv}—La4—La1^{xxvii}	61.370 (13)
In1^{i}—La1—Ru1^{iii}	81.47 (3)	Ru1^{iii}—La4—La1^{xxvii}	119.600 (14)
Ru2^{i}—La1—Ru1^{iii}	81.47 (3)	Ru3^{xxv}—La4—La1^{xxvii}	50.94 (3)
Ru1^{i}—La1—La2^{iv}	103.08 (4)	Ru3^{ii}—La4—La1^{xxvii}	103.96 (4)
Ru3^{ii}—La1—La2^{iv}	125.52 (4)	In1^{i}—La4—La1^{xxvii}	143.53 (3)
Ru4—La1—La2^{iv}	55.00 (3)	In1^{xxv}—La4—La1^{xxvii}	58.39 (2)
In2—La1—La2^{iv}	108.99 (2)	Ru2^{i}—La4—La1^{xxvii}	143.53 (3)
In1^{i}—La1—La2^{iv}	55.539 (19)	Ru2^{xxv}—La4—La1^{xxvii}	58.39 (2)
Ru2^{i}—La1—La2^{iv}	55.539 (19)	La5—La4—La1^{xxvii}	103.13 (2)
Ru1^{iii}—La1—La2^{iv}	46.06 (3)	La3^{iii}—La4—La1^{xxvii}	99.50 (3)
Ru1^{i}—La1—La1^{v}	52.66 (2)	La3^{xvii}—La4—La1^{xxvii}	60.151 (15)
Ru3^{ii}—La1—La1^{v}	52.959 (19)	La1—La4—La1^{xxvii}	153.75 (4)
Ru4—La1—La1^{v}	143.57 (2)	La1^{v}—La4—La1^{xxvii}	115.02 (2)
In2—La1—La1^{v}	138.165 (11)	La1^{xxvi}—La4—La1^{xxvii}	58.26 (2)
In1^{i}—La1—La1^{v}	58.553 (15)	Ru1^{xxiv}—La4—La2^{xxviii}	40.60 (3)
Ru2^{i}—La1—La1^{v}	58.553 (15)	Ru1^{iii}—La4—La2^{xxviii}	136.53 (4)
Ru1^{iii}—La1—La1^{v}	112.56 (3)	Ru3^{xxv}—La4—La2^{xxviii}	102.66 (2)
La2^{iv}—La1—La1^{v}	112.533 (15)	Ru3^{ii}—La4—La2^{xxviii}	131.435 (17)
Ru1^{i}—La1—La4	104.32 (3)	In1^{i}—La4—La2^{xxviii}	91.16 (3)
Ru3^{ii}—La1—La4	55.15 (3)	In1^{xxv}—La4—La2^{xxviii}	49.124 (14)
Ru4—La1—La4	126.43 (3)	Ru2^{i}—La4—La2^{xxviii}	91.16 (3)
In2—La1—La4	141.15 (2)	Ru2^{xxv}—La4—La2^{xxviii}	49.124 (14)
In1^{i}—La1—La4	55.73 (3)	La5—La4—La2^{xxviii}	59.041 (17)
Ru2^{i}—La1—La4	55.73 (3)	La3^{iii}—La4—La2^{xxviii}	151.947 (19)
Ru1^{iii}—La1—La4	51.71 (3)	La3^{xvii}—La4—La2^{xxviii}	82.601 (16)
La2^{iv}—La1—La4	71.84 (2)	La1—La4—La2^{xxviii}	147.12 (2)
La1^{v}—La1—La4	60.869 (10)	La1^{v}—La4—La2^{xxviii}	96.692 (16)
Ru1^{i}—La1—La3^{iii}	152.94 (3)	La1^{xxvi}—La4—La2^{xxviii}	96.726 (16)
Ru3^{ii}—La1—La3^{iii}	51.86 (3)	La1^{xxvii}—La4—La2^{xxviii}	52.689 (13)
Ru4—La1—La3^{iii}	112.87 (3)	Ru1^{xxiv}—La4—La2^{xxv}	40.60 (3)
In2—La1—La3^{iii}	81.52 (2)	Ru1^{iii}—La4—La2^{xxv}	136.53 (4)
In1^{i}—La1—La3^{iii}	113.98 (3)	Ru3^{xxv}—La4—La2^{xxv}	131.435 (17)
Ru2^{i}—La1—La3^{iii}	113.98 (3)	Ru3^{ii}—La4—La2^{xxv}	102.66 (2)
Ru1^{iii}—La1—La3^{iii}	46.85 (3)	In1^{i}—La4—La2^{xxv}	49.124 (14)
La2^{iv}—La1—La3^{iii}	92.826 (19)	In1^{xxv}—La4—La2^{xxv}	91.16 (3)
La1^{v}—La1—La3^{iii}	101.09 (2)	Ru2^{i}—La4—La2^{xxv}	49.124 (14)
La4—La1—La3^{iii}	59.84 (2)	Ru2^{xxv}—La4—La2^{xxv}	91.16 (3)

Ru1^{i}—La1—La2	47.47 (3)	La5—La4—La2^{xxv}	59.041 (17)
Ru3^{ii}—La1—La2	143.25 (3)	La3^{iii}—La4—La2^{xxv}	151.947 (19)
Ru4—La1—La2	53.21 (3)	La3^{xvii}—La4—La2^{xxv}	82.601 (16)
In2—La1—La2	105.542 (19)	La1—La4—La2^{xxv}	96.726 (16)
In1^{i}—La1—La2	52.97 (2)	La1^{v}—La4—La2^{xxv}	52.689 (13)
Ru2^{i}—La1—La2	52.97 (2)	La1^{xxvi}—La4—La2^{xxv}	147.12 (2)
Ru1^{iii}—La1—La2	106.86 (3)	La1^{xxvii}—La4—La2^{xxv}	96.692 (16)
La2^{iv}—La1—La2	60.85 (2)	La2^{xxviii}—La4—La2^{xxv}	50.73 (2)
La1^{v}—La1—La2	90.414 (15)	Ru1^{xxiv}—La4—La2^{iv}	136.53 (4)
La4—La1—La2	107.79 (3)	Ru1^{iii}—La4—La2^{iv}	40.60 (3)
La3^{iii}—La1—La2	153.67 (2)	Ru3^{xxv}—La4—La2^{iv}	131.435 (17)
Ru1^{i}—La1—La1^{vi}	108.52 (3)	Ru3^{ii}—La4—La2^{iv}	102.66 (2)
Ru3^{ii}—La1—La1^{vi}	51.393 (19)	In1^{i}—La4—La2^{iv}	49.124 (14)
Ru4—La1—La1^{vi}	117.89 (3)	In1^{xxv}—La4—La2^{iv}	91.16 (3)
In2—La1—La1^{vi}	54.924 (10)	Ru2^{i}—La4—La2^{iv}	49.124 (14)
In1^{i}—La1—La1^{vi}	147.308 (15)	Ru2^{xxv}—La4—La2^{iv}	91.16 (3)
Ru2^{i}—La1—La1^{vi}	147.308 (15)	La5—La4—La2^{iv}	59.041 (17)
Ru1^{iii}—La1—La1^{vi}	105.49 (3)	La3^{iii}—La4—La2^{iv}	82.601 (16)
La2^{iv}—La1—La1^{vi}	148.189 (14)	La3^{xvii}—La4—La2^{iv}	151.947 (19)
La1^{v}—La1—La1^{vi}	90.0	La1—La4—La2^{iv}	52.689 (13)
La4—La1—La1^{vi}	103.13 (2)	La1^{v}—La4—La2^{iv}	96.726 (16)
La3^{iii}—La1—La1^{vi}	59.766 (9)	La1^{xxvi}—La4—La2^{iv}	96.692 (16)
La2—La1—La1^{vi}	144.697 (13)	La1^{xxvii}—La4—La2^{iv}	147.12 (2)
Ru1^{i}—La1—La1^{iv}	145.48 (3)	La2^{xxviii}—La4—La2^{iv}	118.08 (3)
Ru3^{ii}—La1—La1^{iv}	112.90 (3)	La2^{xxv}—La4—La2^{iv}	95.95 (3)
Ru4—La1—La1^{iv}	51.321 (13)	Ru1^{xxiv}—La4—La2^{i}	136.53 (4)
In2—La1—La1^{iv}	54.641 (5)	Ru1^{iii}—La4—La2^{i}	40.60 (3)
In1^{i}—La1—La1^{iv}	116.06 (2)	Ru3^{xxv}—La4—La2i	102.66 (2)
Ru2^{i}—La1—La1^{iv}	116.06 (2)	Ru3i—La4—La2i	131.435 (17)
Ru1^{iii}—La1—La1^{iv}	47.96 (3)	In1i—La4—La2i	91.16 (3)
La2^{iv}—La1—La1^{iv}	60.927 (16)	In1i—La4—La2i	49.124 (14)
La1^{v}—La1—La1^{iv}	159.439 (14)	Ru2i—La4—La2i	91.16 (3)
La4—La1—La1^{iv}	99.18 (2)	Ru2i—La4—La2i	49.124 (14)
La3^{iii}—La1—La1^{iv}	61.58 (3)	La5—La4—La2i	59.041 (17)
La2—La1—La1^{iv}	101.314 (14)	La3i—La4—La2i	82.601 (16)
La1^{vi}—La1—La1^{iv}	90.0	La3i—La4—La2i	151.947 (19)
Ru1^{i}—La1—La1^{vii}	62.01 (3)	La1—La4—La2i	96.692 (16)
Ru3^{ii}—La1—La1^{vii}	132.66 (4)	La1i—La4—La2i	147.12 (2)
Ru4—La1—La1^{vii}	51.321 (13)	La1i—La4—La2i	52.689 (13)
In2—La1—La1^{vii}	54.641 (5)	La1i—La4—La2i	96.726 (16)
In1^{i}—La1—La1^{vii}	108.31 (3)	La2i—La4—La2i	95.95 (3)

Ru2^{i}—La1—La1^{vii}	108.31 (3)	La2i—La4—La2i	118.08 (3)
Ru1^{iii}—La1—La1^{vii}	133.87 (3)	La2i—La4—La2i	50.73 (2)
La2^{iv}—La1—La1^{vii}	101.787 (14)	In1i—La5—Ru2i	0.00 (5)
La1^{v}—La1—La1^{vii}	110.561 (14)	In1i—La5—In1i	116.87 (4)
La4—La1—La1^{vii}	163.89 (2)	Ru2i—La5—In1i	116.87 (4)
La3^{iii}—La1—La1^{vii}	136.140 (19)	In1i—La5—Ru2i	116.87 (4)
La2—La1—La1^{vii}	57.072 (15)	Ru2i—La5—Ru2i	116.87 (4)
La1^{vi}—La1—La1^{vii}	90.0	In1i—La5—Ru2i	0.00 (5)
La1^{iv}—La1—La1^{vii}	90.0	In1i—La5—In1i	105.90 (2)
Ru1^{i}—La1—La3^{ii}	48.24 (4)	Ru2i—La5—In1i	105.90 (2)
Ru3^{ii}—La1—La3^{ii}	77.10 (4)	In1i—La5—In1i	105.90 (2)
Ru4—La1—La3^{ii}	109.84 (2)	Ru2i—La5—In1i	105.90 (2)
In2—La1—La3^{ii}	79.748 (13)	In1i—La5—In1i	105.90 (2)
In1^{i}—La1—La3^{ii}	105.53 (2)	Ru2i—La5—In1i	105.90 (2)
Ru2^{i}—La1—La3^{ii}	105.53 (2)	In1i—La5—In1i	105.90 (2)
Ru1^{iii}—La1—La3^{ii}	163.83 (3)	Ru2i—La5—In1i	105.90 (2)
La2^{iv}—La1—La3^{ii}	149.48 (2)	In1i—La5—In1i	116.87 (4)
La1^{v}—La1—La3^{ii}	61.869 (12)	In1i—La5—Ru2i	105.90 (2)
La4—La1—La3^{ii}	120.05 (2)	Ru2i—La5—Ru2i	105.90 (2)
La3^{iii}—La1—La3^{ii}	117.600 (15)	In1i—La5—Ru2i	105.90 (2)
La2—La1—La3^{ii}	88.72 (2)	Ru2i—La5—Ru2i	105.90 (2)
La1^{vi}—La1—La3^{ii}	60.766 (12)	In1i—La5—Ru2i	0.00 (5)
La1^{iv}—La1—La3^{ii}	134.374 (13)	In1i—La5—Ru2i	116.87 (4)
La1^{vii}—La1—La3^{ii}	58.54 (2)	In1i—La5—Ru2i	105.90 (2)
Ru1^{i}—La2—Ru5	153.94 (4)	Ru2i—La5—Ru2i	105.90 (2)
Ru1^{i}—La2—Ru4	96.58 (4)	In1i—La5—Ru2i	105.90 (2)
Ru5—La2—Ru4	61.66 (3)	Ru2i—La5—Ru2i	105.90 (2)
Ru1^{i}—La2—In1^{i}	66.35 (5)	In1i—La5—Ru2i	116.87 (4)
Ru5—La2—In1^{i}	100.77 (3)	In1i—La5—Ru2i	0.00 (5)
Ru4—La2—In1^{i}	98.14 (2)	Ru2i—La5—Ru2i	116.87 (4)
Ru1^{i}—La2—Ru2^{i}	66.35 (5)	In1i—La5—La4i	58.44 (2)
Ru5—La2—Ru2^{i}	100.77 (3)	Ru2i—La5—La4i	58.44 (2)
Ru4—La2—Ru2^{i}	98.14 (2)	In1i—La5—La4i	58.44 (2)
In1^{i}—La2—Ru2^{i}	0.00 (5)	Ru2i—La5—La4i	58.44 (2)
Ru1^{i}—La2—In1^{viii}	97.34 (5)	In1i—La5—La4i	121.56 (2)
Ru5—La2—In1^{viii}	99.26 (3)	In1i—La5—La4i	121.56 (2)
Ru4—La2—In1^{viii}	96.72 (3)	Ru2i—La5—La4i	121.56 (2)
In1^{i}—La2—In1^{viii}	159.05 (3)	Ru2i—La5—La4i	121.56 (2)
Ru2^{i}—La2—In1^{viii}	159.05 (3)	In1i—La5—La4	121.56 (2)
Ru1^{i}—La2—Ru2^{viii}	97.34 (5)	Ru2i—La5—La4	121.56 (2)
Ru5—La2—Ru2^{viii}	99.26 (3)	In1i—La5—La4	121.56 (2)

Ru4—La2—Ru2^{viii}	96.72 (3)	Ru2i—La5—La4	121.56 (2)
In1^{i}—La2—Ru2^{viii}	159.05 (3)	In1i—La5—La4	58.44 (2)
Ru2^{i}—La2—Ru2^{viii}	159.05 (3)	In1i—La5—La4	58.44 (2)
In1^{viii}—La2—Ru2^{viii}	0.00 (5)	Ru2i—La5—La4	58.44 (2)
Ru1^{i}—La2—La2^{ix}	152.02 (3)	Ru2i—La5—La4	58.44 (2)
Ru5—La2—La2^{ix}	54.020 (13)	La4i—La5—La4	180.0
Ru4—La2—La2^{ix}	106.31 (3)	In1i—La5—La2i	151.770 (11)
In1^{i}—La2—La2^{ix}	124.21 (4)	Ru2i—La5—La2i	151.770 (11)
Ru2^{i}—La2—La2^{ix}	124.21 (4)	In1i—La5—La2i	60.91 (2)
In1^{viii}—La2—La2^{ix}	64.66 (3)	Ru2i—La5—La2i	60.91 (2)
Ru2^{viii}—La2—La2^{ix}	64.66 (3)	In1i—La5—La2i	101.346 (16)
Ru1^{i}—La2—La1^{vii}	66.18 (3)	In1i—La5—La2i	53.724 (10)
Ru5—La2—La1^{vii}	105.49 (2)	Ru2i—La5—La2i	101.346 (16)
Ru4—La2—La1^{vii}	53.12 (3)	Ru2i—La5—La2i	53.724 (10)
In1^{i}—La2—La1^{vii}	119.10 (3)	La4i—La5—La2i	112.164 (9)
Ru2^{i}—La2—La1^{vii}	119.10 (3)	La4—La5—La2i	67.836 (9)
In1^{viii}—La2—La1^{vii}	60.38 (3)	In1i—La5—La2i	151.770 (11)
Ru2^{viii}—La2—La1^{vii}	60.38 (3)	Ru2i—La5—La2i	151.770 (11)
La2^{ix}—La2—La1^{vii}	115.72 (3)	In1i—La5—La2i	60.91 (2)
Ru1^{i}—La2—La2^{x}	128.22 (4)	Ru2i—La5—La2i	60.91 (2)
Ru5—La2—La2^{x}	52.682 (13)	In1i—La5—La2i	53.724 (10)
Ru4—La2—La2^{x}	103.66 (3)	In1i—La5—La2i	101.346 (16)
In1^{i}—La2—La2^{x}	63.93 (3)	Ru2i—La5—La2i	53.724 (10)
Ru2^{i}—La2—La2^{x}	63.93 (3)	Ru2i—La5—La2i	101.346 (16)
In1^{viii}—La2—La2^{x}	126.15 (4)	La4i—La5—La2i	112.164 (9)
Ru2^{viii}—La2—La2^{x}	126.15 (4)	La4—La5—La2i	67.836 (9)
La2^{ix}—La2—La2^{x}	61.90 (2)	La2i—La5—La2i	55.12 (2)
La1^{vii}—La2—La2^{x}	156.27 (2)	In1i—La5—La2i	53.724 (10)
Ru1^{i}—La2—In1^{xi}	108.17 (3)	Ru2i—La5—La2i	53.724 (10)
Ru5—La2—In1^{xi}	91.53 (2)	In1i—La5—La2i	101.346 (16)
Ru4—La2—In1^{xi}	152.93 (4)	Ru2i—La5—La2i	101.346 (16)
In1^{i}—La2—In1^{xi}	82.45 (3)	In1i—La5—La2i	151.770 (11)
Ru2^{i}—La2—In1^{xi}	82.45 (3)	In1i—La5—La2i	60.91 (2)
In1^{viii}—La2—In1^{xi}	90.96 (4)	Ru2i—La5—La2i	151.770 (11)
Ru2^{viii}—La2—In1^{xi}	90.96 (4)	Ru2i—La5—La2i	60.91 (2)
La2^{ix}—La2—In1^{xi}	54.223 (18)	La4i—La5—La2i	67.836 (9)
La1^{vii}—La2—In1^{xi}	148.25 (3)	La4—La5—La2i	112.164 (9)
La2^{x}—La2—In1^{xi}	52.17 (2)	La2i—La5—La2i	98.183 (7)
Ru1^{i}—La2—Ru2^{xi}	108.17 (3)	La2i—La5—La2i	152.21 (2)
Ru5—La2—Ru2^{xi}	91.53 (2)	In1i—La5—La2i	53.724 (10)
Ru4—La2—Ru2^{xi}	152.93 (4)	Ru2i—La5—La2i	53.724 (10)

$In1^{i}$—La2—$Ru2^{xi}$	82.45 (3)	In1i—La5—La2i	101.346 (16)
$Ru2^{i}$—La2—$Ru2^{xi}$	82.45 (3)	Ru2i—La5—La2i	101.346 (16)
$In1^{viii}$—La2—$Ru2^{xi}$	90.96 (4)	In1i—La5—La2i	60.91 (2)
$Ru2^{viii}$—La2—$Ru2^{xi}$	90.96 (4)	In1i—La5—La2i	151.770 (11)
$La2^{ix}$—La2—$Ru2^{xi}$	54.223 (18)	Ru2i—La5—La2i	60.91 (2)
$La1^{vii}$—La2—$Ru2^{xi}$	148.25 (3)	Ru2i—La5—La2i	151.770 (11)
$La2^{x}$—La2—$Ru2^{xi}$	52.17 (2)	La4i—La5—La2i	67.836 (9)
$In1^{xi}$—La2—$Ru2^{xi}$	0.00 (2)	La4—La5—La2i	112.164 (9)
$Ru1^{i}$—La2—$La2^{v}$	48.86 (3)	La2i—La5—La2i	152.21 (2)
Ru5—La2—$La2^{v}$	142.682 (13)	La2i—La5—La2i	98.183 (7)
Ru4—La2—$La2^{v}$	140.98 (2)	La2i—La5—La2i	106.69 (2)
$In1^{i}$—La2—$La2^{v}$	55.251 (18)	In1i—La5—La2i	60.91 (2)
$Ru2^{i}$—La2—$La2^{v}$	55.251 (18)	Ru2i—La5—La2i	60.91 (2)
$In1^{viii}$—La2—$La2^{v}$	104.32 (2)	In1i—La5—La2i	151.770 (11)
$Ru2^{viii}$—La2—$La2^{v}$	104.32 (2)	Ru2i—La5—La2i	151.770 (11)
$La2^{ix}$—La2—$La2^{v}$	112.316 (14)	In1i—La5—La2i	101.346 (16)
$La1^{vii}$—La2—$La2^{v}$	111.218 (15)	In1i—La5—La2i	53.724 (10)
$La2^{x}$—La2—$La2^{v}$	90.0	Ru2i—La5—La2i	101.346 (16)
$In1^{xi}$—La2—$La2^{v}$	59.923 (14)	Ru2i—La5—La2i	53.724 (10)
$Ru2^{xi}$—La2—$La2^{v}$	59.923 (14)	La4i—La5—La2i	112.164 (9)
$Ru1^{i}$—La2—$La2^{vii}$	127.67 (3)	La4—La5—La2i	67.836 (9)
Ru5—La2—$La2^{vii}$	52.110 (5)	La2i—La5—La2i	106.69 (2)
Ru4—La2—$La2^{vii}$	53.130 (14)	La2i—La5—La2i	135.671 (18)
$In1^{i}$—La2—$La2^{vii}$	146.01 (3)	La2i—La5—La2i	53.130 (19)
$Ru2^{i}$—La2—$La2^{vii}$	146.01 (3)	La2i—La5—La2i	98.183 (7)
$In1^{viii}$—La2—$La2^{vii}$	54.40 (3)	In1i—La5—La2i	60.91 (2)
$Ru2^{viii}$—La2—$La2^{vii}$	54.40 (3)	Ru2i—La5—La2i	60.91 (2)
$La2^{ix}$—La2—$La2^{vii}$	60.55 (2)	In1i—La5—La2i	151.770 (11)
$La1^{vii}$—La2—$La2^{vii}$	61.549 (16)	Ru2i—La5—La2i	151.770 (11)
$La2^{x}$—La2—$La2^{vii}$	102.075 (5)	In1i—La5—La2i	53.724 (10)
$In1^{xi}$—La2—$La2^{vii}$	114.454 (19)	In1i—La5—La2i	101.346 (16)
$Ru2^{xi}$—La2—$La2^{vii}$	114.454 (19)	Ru2i—La5—La2i	53.724 (10)
$La2^{v}$—La2—$La2^{vii}$	158.701 (16)	Ru2i—La5—La2i	101.346 (16)
$Ru1^{i}$—La2—$La2^{iv}$	104.12 (4)	La4i—La5—La2i	112.164 (9)
Ru5—La2—$La2^{iv}$	52.110 (5)	La4—La5—La2i	67.836 (9)
Ru4—La2—$La2^{iv}$	53.130 (14)	La2i—La5—La2i	135.671 (18)
$In1^{i}$—La2—$La2^{iv}$	56.11 (3)	La2i—La5—La2i	106.69 (2)
$Ru2^{i}$—La2—$La2^{iv}$	56.11 (3)	La2i—La5—La2i	98.183 (7)
$In1^{viii}$—La2—$La2^{iv}$	144.30 (3)	La2i—La5—La2i	53.130 (19)
$Ru2^{viii}$—La2—$La2^{iv}$	144.30 (3)	La2i—La5—La2i	55.12 (2)
$La2^{ix}$—La2—$La2^{iv}$	102.465 (5)	In1i—La5—La2i	101.346 (16)

La1^{vii}—La2—La2^{iv}	103.037 (14)	Ru2i—La5—La2i	101.346 (16)
La2^{x}—La2—La2^{iv}	57.55 (2)	In1i—La5—La2i	53.724 (10)
In1^{xi}—La2—La2^{iv}	108.54 (3)	Ru2i—La5—La2i	53.724 (10)
Ru2^{xi}—La2—La2^{iv}	108.54 (3)	In1i—La5—La2i	151.770 (11)
La2^{v}—La2—La2^{iv}	111.299 (16)	In1i—La5—La2i	60.91 (2)
La2^{vii}—La2—La2^{iv}	90.0	Ru2i—La5—La2i	151.770 (11)
Ru1^{i}—La2—La1	51.96 (3)	Ru2i—La5—La2i	60.91 (2)
Ru5—La2—La1	102.03 (2)	La4i—La5—La2i	67.836 (9)
Ru4—La2—La1	51.44 (2)	La4—La5—La2i	112.164 (9)
In1^{i}—La2—La1	59.24 (3)	La2i—La5—La2i	53.130 (19)
Ru2^{i}—La2—La1	59.24 (3)	La2i—La5—La2i	98.183 (7)
In1^{viii}—La2—La1	121.93 (3)	La2i—La5—La2i	55.12 (2)
Ru2^{viii}—La2—La1	121.93 (3)	La2i—La5—La2i	135.671 (18)
La2^{ix}—La2—La1	155.591 (17)	La2i—La5—La2i	98.183 (7)
La1^{vii}—La2—La1	62.001 (19)	La2i—La5—La2i	152.21 (2)
La2^{x}—La2—La1	109.54 (3)	In1i—La5—La2i	101.346 (16)
In1^{xi}—La2—La1	140.96 (3)	Ru2i—La5—La2i	101.346 (16)
Ru2^{xi}—La2—La1	140.96 (3)	In1i—La5—La2i	53.724 (10)
La2^{v}—La2—La1	89.586 (15)	Ru2i—La5—La2i	53.724 (10)
La2^{vii}—La2—La1	102.512 (13)	In1i—La5—La2i	60.91 (2)
La2^{iv}—La2—La1	57.604 (16)	In1i—La5—La2i	151.770 (11)
Ru1^{i}—La2—La5^{xii}	88.59 (4)	Ru2i—La5—La2i	60.91 (2)
Ru5—La2—La5^{xii}	117.455 (19)	Ru2i—La5—La2i	151.770 (11)
Ru4—La2—La5^{xii}	146.38 (2)	La4i—La5—La2i	67.836 (9)
In1^{i}—La2—La5^{xii}	114.20 (2)	La4—La5—La2i	112.164 (9)
Ru2^{i}—La2—La5^{xii}	114.20 (2)	La2i—La5—La2i	98.183 (7)
In1^{viii}—La2—La5^{xii}	49.67 (2)	La2i—La5—La2i	53.130 (19)
Ru2^{viii}—La2—La5^{xii}	49.67 (2)	La2i—La5—La2i	135.671 (18)
La2^{ix}—La2—La5^{xii}	63.435 (9)	La2i—La5—La2i	55.12 (2)
La1^{vii}—La2—La5^{xii}	100.404 (19)	La2i—La5—La2i	152.21 (2)
La2^{x}—La2—La5^{xii}	98.84 (2)	La2i—La5—La2i	98.183 (7)
In1^{xi}—La2—La5^{xii}	47.88 (2)	La2i—La5—La2i	106.69 (2)
Ru2^{xi}—La2—La5^{xii}	47.88 (2)	La2i—Ru1—La2i	82.28 (5)
La2^{v}—La2—La5^{xii}	62.442 (10)	La2i—Ru1—La3	137.34 (3)
La2^{vii}—La2—La5^{xii}	98.03 (2)	La2i—Ru1—La3	137.34 (3)
La2^{iv}—La2—La5^{xii}	156.280 (13)	La2i—Ru1—La1i	129.38 (7)
La1—La2—La5^{xii}	140.19 (2)	La2i—Ru1—La1i	80.57 (3)
Ru1^{i}—La2—La4^{xiii}	47.69 (4)	La3—Ru1—La1i	81.52 (4)
Ru5—La2—La4^{xiii}	148.76 (2)	La2i—Ru1—La1i	80.57 (3)
Ru4—La2—La4^{xiii}	108.30 (3)	La2i—Ru1—La1i	129.38 (7)
In1^{i}—La2—La4^{xiii}	110.16 (3)	La3—Ru1—La1i	81.52 (4)

$Ru2^{i}$—La2—$La4^{xiii}$	110.16 (3)	La1i—Ru1—La1i	74.69 (5)
$In1^{viii}$—La2—$La4^{xiii}$	50.68 (2)	La2i—Ru1—La4i	91.71 (5)
$Ru2^{viii}$—La2—$La4^{xiii}$	50.68 (2)	La2i—Ru1—La4i	91.71 (5)
$La2^{ix}$—La2—$La4^{xiii}$	108.33 (2)	La3—Ru1—La4i	75.27 (6)
$La1^{vii}$—La2—$La4^{xiii}$	55.473 (19)	La1i—Ru1—La4i	135.90 (4)
$La2^{x}$—La2—$La4^{xiii}$	148.03 (2)	La1i—Ru1—La4i	135.90 (4)
$In1^{xi}$—La2—$La4^{xiii}$	96.65 (3)	La2i—Ru1—La1i	67.76 (2)
$Ru2^{xi}$—La2—$La4^{xiii}$	96.65 (3)	La2i—Ru1—La1i	141.71 (5)
$La2^{v}$—La2—$La4^{xiii}$	64.635 (10)	La3—Ru1—La1i	69.77 (3)
$La2^{vii}$—La2—$La4^{xiii}$	97.43 (2)	La1i—Ru1—La1i	136.97 (5)
$La2^{iv}$—La2—$La4^{xiii}$	147.966 (18)	La1i—Ru1—La1i	70.03 (2)
La1—La2—$La4^{xiii}$	90.36 (2)	La4i—Ru1—La1i	66.92 (3)
$La5^{xii}$—La2—$La4^{xiii}$	53.123 (17)	La2i—Ru1—La1i	141.71 (5)
$Ru1^{vi}$—La3—Ru1	154.28 (9)	La2i—Ru1—La1i	67.76 (2)
$Ru1^{vi}$—La3—$Ru3^{xiv}$	100.76 (4)	La3—Ru1—La1i	69.77 (3)
Ru1—La3—$Ru3^{xiv}$	100.76 (4)	La1i—Ru1—La1i	70.03 (2)
$Ru1^{vi}$—La3—$Ru3^{xv}$	100.76 (4)	La1i—Ru1—La1i	136.97 (5)
Ru1—La3—$Ru3^{xv}$	100.76 (4)	La4i—Ru1—La1i	66.92 (3)
$Ru3^{xiv}$—La3—$Ru3^{xv}$	65.99 (7)	La1i—Ru1—La1i	124.26 (6)
$Ru1^{vi}$—La3—$La4^{xvi}$	149.96 (5)	La5i—Ru2—La2i	132.69 (3)
Ru1—La3—$La4^{xvi}$	55.75 (4)	La5i—Ru2—La2i	132.69 (3)
$Ru3^{xiv}$—La3—$La4^{xvi}$	55.19 (2)	La2i—Ru2—La2i	69.50 (4)
$Ru3^{xv}$—La3—$La4^{xvi}$	55.19 (2)	La5i—Ru2—La2i	76.61 (3)
$Ru1^{vi}$—La3—$La4^{xvii}$	55.75 (4)	La2i—Ru2—La2i	69.49 (3)
Ru1—La3—$La4^{xvii}$	149.96 (5)	La2i—Ru2—La2i	138.87 (3)
$Ru3^{xiv}$—La3—$La4^{xvii}$	55.19 (2)	La5i—Ru2—La2i	76.61 (3)
$Ru3^{xv}$—La3—$La4^{xvii}$	55.19 (2)	La2i—Ru2—La2i	138.87 (3)
$La4^{xvi}$—La3—$La4^{xvii}$	94.21 (4)	La2i—Ru2—La2i	69.49 (3)
$Ru1^{vi}$—La3—$La1^{xvi}$	122.257 (9)	La2i—Ru2—La2i	150.98 (5)
Ru1—La3—$La1^{xvi}$	63.380 (15)	La5i—Ru2—La4i	69.62 (3)
$Ru3^{xiv}$—La3—$La1^{xvi}$	51.68 (3)	La2i—Ru2—La4i	132.16 (3)
$Ru3^{xv}$—La3—$La1^{xvi}$	107.30 (4)	La2i—Ru2—La4i	132.16 (3)
$La4^{xvi}$—La3—$La1^{xvi}$	60.009 (14)	La2i—Ru2—La4i	80.19 (2)
$La4^{xvii}$—La3—$La1^{xvi}$	103.76 (3)	La2i—Ru2—La4i	80.19 (2)
$Ru1^{vi}$—La3—$La1^{xviii}$	63.380 (15)	La5i—Ru2—La1i	124.03 (3)
Ru1—La3—$La1^{xviii}$	122.257 (9)	La2i—Ru2—La1i	67.79 (3)
$Ru3^{xiv}$—La3—$La1^{xviii}$	107.30 (4)	La2i—Ru2—La1i	102.52 (4)
$Ru3^{xv}$—La3—$La1^{xviii}$	51.68 (3)	La2i—Ru2—La1i	64.082 (19)
$La4^{xvi}$—La3—$La1^{xviii}$	103.76 (3)	La2i—Ru2—La1i	124.96 (4)
$La4^{xvii}$—La3—$La1^{xviii}$	60.009 (14)	La4i—Ru2—La1i	65.88 (3)
$La1^{xvi}$—La3—$La1^{xviii}$	157.81 (4)	La5i—Ru2—La1i	124.03 (3)

Ru1^{vi}—La3—La1^{xix}	63.380 (15)	La2i—Ru2—La1i	102.52 (4)
Ru1—La3—La1^{xix}	122.257 (9)	La2i—Ru2—La1i	67.79 (3)
Ru3^{xiv}—La3—La1^{xix}	51.68 (3)	La2i—Ru2—La1i	124.96 (4)
Ru3^{xv}—La3—La1^{xix}	107.30 (4)	La2i—Ru2—La1i	64.082 (19)
La4^{xvi}—La3—La1^{xix}	103.76 (3)	La4i—Ru2—La1i	65.88 (3)
La4^{xvii}—La3—La1^{xix}	60.009 (14)	La1i—Ru2—La1i	62.89 (3)
La1^{xvi}—La3—La1^{xix}	60.467 (19)	La5i—Ru2—La2i	71.20 (3)
La1^{xviii}—La3—La1^{xix}	114.76 (2)	La2i—Ru2—La2i	63.90 (3)
Ru1^{vi}—La3—La1^{xx}	122.257 (9)	La2i—Ru2—La2i	97.55 (3)
Ru1—La3—La1^{xx}	63.380 (15)	La2i—Ru2—La2i	61.12 (2)
Ru3^{xiv}—La3—La1^{xx}	107.30 (4)	La2i—Ru2—La2i	119.17 (4)
Ru3^{xv}—La3—La1^{xx}	51.68 (3)	La4i—Ru2—La2i	129.84 (4)
La4^{xvi}—La3—La1^{xx}	60.009 (14)	La1i—Ru2—La2i	115.849 (17)
La4^{xvii}—La3—La1^{xx}	103.76 (3)	La1i—Ru2—La2i	163.52 (4)
La1^{xvi}—La3—La1^{xx}	114.76 (2)	La5i—Ru2—La2i	71.20 (3)
La1^{xviii}—La3—La1^{xx}	60.467 (19)	La2i—Ru2—La2i	97.55 (3)
La1^{xix}—La3—La1^{xx}	157.81 (4)	La2i—Ru2—La2i	63.90 (3)
Ru1^{vi}—La3—La1^{xiv}	50.24 (3)	La2i—Ru2—La2i	119.17 (4)
Ru1—La3—La1^{xiv}	108.22 (4)	La2i—Ru2—La2i	61.12 (2)
Ru3^{xiv}—La3—La1^{xiv}	150.765 (12)	La4i—Ru2—La2i	129.84 (4)
Ru3^{xv}—La3—La1^{xiv}	111.05 (3)	La1i—Ru2—La2i	163.52 (4)
La4^{xvi}—La3—La1^{xiv}	149.047 (11)	La1i—Ru2—La2i	115.849 (17)
La4^{xvii}—La3—La1^{xiv}	98.166 (15)	La2i—Ru2—La2i	60.15 (3)
La1^{xvi}—La3—La1^{xiv}	141.66 (3)	La1i—Ru3—La1i	77.21 (4)
La1^{xviii}—La3—La1^{xiv}	59.886 (19)	La1i—Ru3—La1i	120.29 (7)
La1^{xix}—La3—La1^{xiv}	107.008 (19)	La1i—Ru3—La1i	74.08 (4)
La1^{xx}—La3—La1^{xiv}	89.43 (2)	La1i—Ru3—La1i	74.08 (4)
Ru1^{vi}—La3—La1^{xxi}	50.24 (3)	La1i—Ru3—La1i	120.29 (7)
Ru1—La3—La1^{xxi}	108.22 (4)	La1i—Ru3—La1i	77.21 (4)
Ru3^{xiv}—La3—La1^{xxi}	111.04 (3)	La1i—Ru3—La3i	76.459 (16)
Ru3^{xv}—La3—La1^{xxi}	150.765 (12)	La1i—Ru3—La3i	76.459 (16)
La4^{xvi}—La3—La1^{xxi}	149.047 (11)	La1i—Ru3—La3i	140.924 (12)
La4^{xvii}—La3—La1^{xxi}	98.166 (15)	La1i—Ru3—La3i	140.924 (12)
La1^{xvi}—La3—La1^{xxi}	89.43 (2)	La1i—Ru3—La3i	140.924 (12)
La1^{xviii}—La3—La1^{xxi}	107.008 (19)	La1i—Ru3—La3i	140.924 (12)
La1^{xix}—La3—La1^{xxi}	59.886 (19)	La1i—Ru3—La3i	76.459 (16)
La1^{xx}—La3—La1^{xxi}	141.66 (3)	La1i—Ru3—La3i	76.459 (16)
La1^{xiv}—La3—La1^{xxi}	56.26 (2)	La3i—Ru3—La3i	114.01 (7)
Ru1^{vi}—La3—La1^{xxii}	108.22 (4)	La1i—Ru3—La4i	73.911 (15)
Ru1—La3—La1^{xxii}	50.24 (3)	La1i—Ru3—La4i	142.318 (12)
Ru3^{xiv}—La3—La1^{xxii}	150.765 (12)	La1i—Ru3—La4i	142.317 (12)

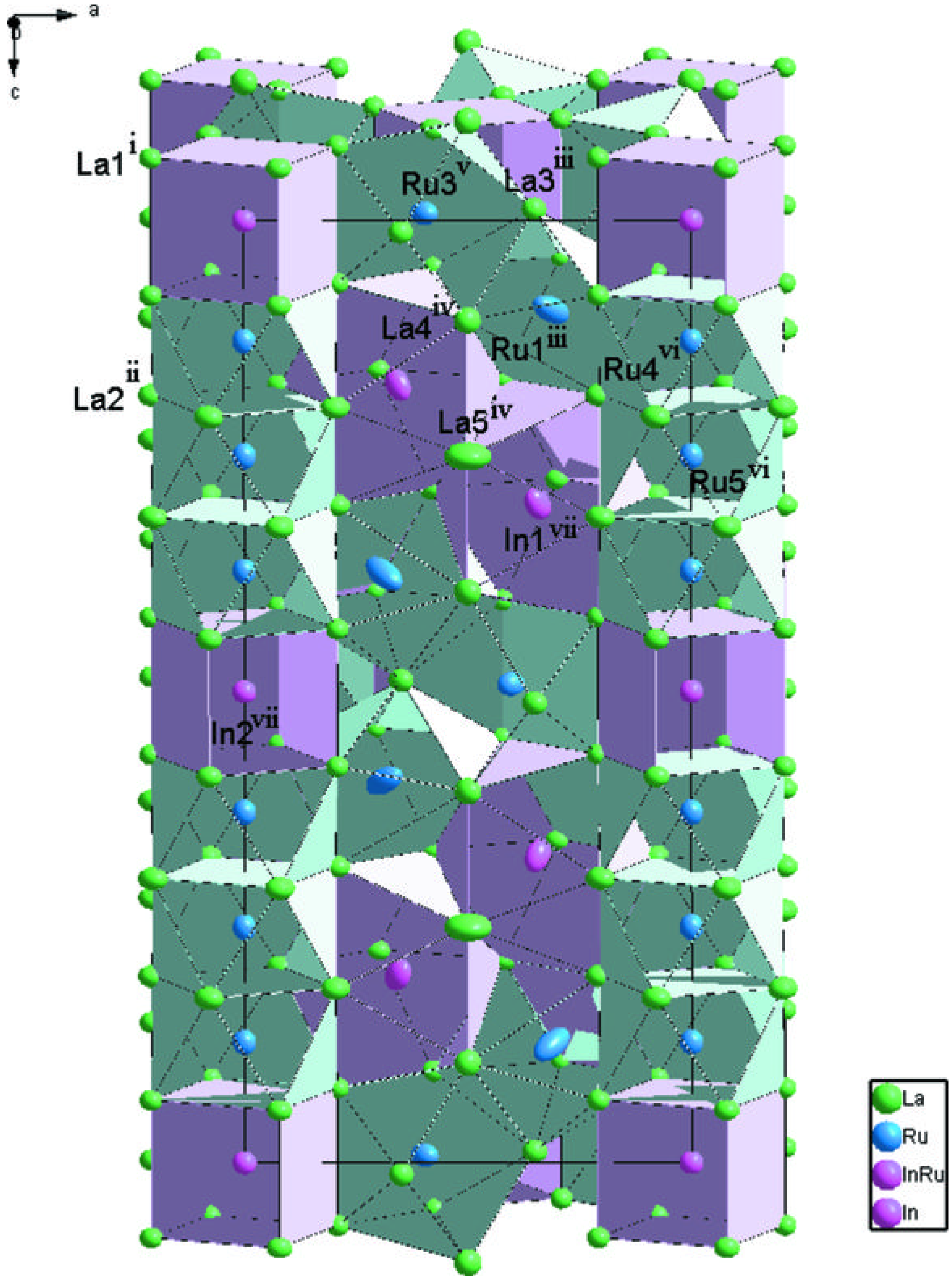
$Ru3^{xv}$—La3—$La1^{xxii}$	111.05 (3)	La1i—Ru3—La4i	73.911 (15)
$La4^{xvi}$—La3—$La1^{xxii}$	98.166 (15)	La3i—Ru3—La4i	73.66 (3)
$La4^{xvii}$—La3—$La1^{xxii}$	149.047 (11)	La3i—Ru3—La4i	73.66 (3)
$La1^{xvi}$—La3—$La1^{xxii}$	107.008 (19)	La1i—Ru3—La4i	142.317 (12)
$La1^{xviii}$—La3—$La1^{xxii}$	89.43 (2)	La1i—Ru3—La4i	73.911 (15)
$La1^{xix}$—La3—$La1^{xxii}$	141.66 (3)	La1i—Ru3—La4i	73.911 (15)
$La1^{xx}$—La3—$La1^{xxii}$	59.886 (19)	La1i—Ru3—La4i	142.318 (12)
$La1^{xiv}$—La3—$La1^{xxii}$	58.47 (2)	La3i—Ru3—La4i	73.66 (3)
$La1^{xxi}$—La3—$La1^{xxii}$	85.50 (3)	La3i—Ru3—La4i	73.66 (3)
$Ru1^{vi}$—La3—$La1^{xxiii}$	108.22 (4)	La4i—Ru3—La4i	117.80 (7)
Ru1—La3—$La1^{xxiii}$	50.24 (3)	La1i—Ru4—La1i	77.36 (3)
$Ru3^{xiv}$—La3—$La1^{xxiii}$	111.04 (3)	La1i—Ru4—La1	124.21 (6)
$Ru3^{xv}$—La3—$La1^{xxiii}$	150.765 (12)	La1i—Ru4—La1	77.36 (3)
$La4^{xvi}$—La3—$La1^{xxiii}$	98.166 (15)	La1i—Ru4—La1i	77.36 (3)
$La4^{xvii}$—La3—$La1^{xxiii}$	149.047 (11)	La1i—Ru4—La1i	124.21 (6)
$La1^{xvi}$—La3—$La1^{xxiii}$	59.886 (19)	La1—Ru4—La1i	77.36 (3)
$La1^{xviii}$—La3—$La1^{xxiii}$	141.66 (3)	La1i—Ru4—La2	138.418 (17)
$La1^{xix}$—La3—$La1^{xxiii}$	89.43 (2)	La1i—Ru4—La2	143.716 (18)
$La1^{xx}$—La3—$La1^{xxiii}$	107.008 (19)	La1—Ru4—La2	75.350 (16)
$La1^{xiv}$—La3—$La1^{xxiii}$	85.50 (3)	La1i—Ru4—La2	71.881 (16)
$La1^{xxi}$—La3—$La1^{xxiii}$	58.47 (2)	La1i—Ru4—La2i	143.716 (18)
$La1^{xxii}$—La3—$La1^{xxiii}$	56.26 (2)	La1i—Ru4—La2i	75.350 (16)
$Ru1^{xxiv}$—La4—$Ru1^{iii}$	176.27 (8)	La1—Ru4—La2i	71.881 (16)
$Ru1^{xxiv}$—La4—$Ru3^{xxv}$	91.60 (3)	La1i—Ru4—La2i	138.418 (17)
$Ru1^{iii}$—La4—$Ru3^{xxv}$	91.60 (3)	La2—Ru4—La2i	73.74 (3)
$Ru1^{xxiv}$—La4—$Ru3^{ii}$	91.60 (3)	La1i—Ru4—La2i	75.350 (16)
$Ru1^{iii}$—La4—$Ru3^{ii}$	91.60 (3)	La1i—Ru4—La2i	71.881 (16)
$Ru3^{xxv}$—La4—$Ru3^{ii}$	62.20 (7)	La1—Ru4—La2i	138.418 (17)
$Ru1^{xxiv}$—La4—$In1^{i}$	88.85 (2)	La1i—Ru4—La2i	143.716 (18)
$Ru1^{iii}$—La4—$In1^{i}$	88.85 (2)	La2—Ru4—La2i	116.11 (6)
$Ru3^{xxv}$—La4—$In1^{i}$	159.16 (5)	La2i—Ru4—La2i	73.74 (3)
$Ru3^{ii}$—La4—$In1^{i}$	96.95 (4)	La1i—Ru4—La2i	71.881 (16)
$Ru1^{xxiv}$—La4—$In1^{xxv}$	88.85 (2)	La1i—Ru4—La2i	138.418 (17)
$Ru1^{iii}$—La4—$In1^{xxv}$	88.85 (2)	La1—Ru4—La2i	143.716 (18)
$Ru3^{xxv}$—La4—$In1^{xxv}$	96.95 (4)	La1i—Ru4—La2i	75.350 (16)
$Ru3^{ii}$—La4—$In1^{xxv}$	159.16 (5)	La2—Ru4—La2i	73.74 (3)
$In1^{i}$—La4—$In1^{xxv}$	103.89 (6)	La2i—Ru4—La2i	116.11 (6)
$Ru1^{xxiv}$—La4—$Ru2^{i}$	88.85 (2)	La2i—Ru4—La2i	73.74 (3)
$Ru1^{iii}$—La4—$Ru2^{i}$	88.85 (2)	La2i—Ru5—La2i	139.13 (3)
$Ru3^{xxv}$—La4—$Ru2^{i}$	159.16 (5)	La2i—Ru5—La2i	143.22 (3)
$Ru3^{ii}$—La4—$Ru2^{i}$	96.95 (4)	La2i—Ru5—La2i	75.781 (11)

$In1^{i}$—La4—$Ru2^{i}$	0.00 (4)	La2i—Ru5—La2i	75.781 (11)
$In1^{xxv}$—La4—$Ru2^{i}$	103.89 (6)	La2i—Ru5—La2i	143.22 (3)
$Ru1^{xxiv}$—La4—$Ru2^{xxv}$	88.85 (2)	La2i—Ru5—La2i	74.64 (3)
$Ru1^{iii}$—La4—$Ru2^{xxv}$	88.85 (2)	La2i—Ru5—La2i	120.58 (2)
$Ru3^{xxv}$—La4—$Ru2^{xxv}$	96.95 (4)	La2i—Ru5—La2i	74.64 (3)
$Ru3^{ii}$—La4—$Ru2^{xxv}$	159.16 (5)	La2i—Ru5—La2i	71.96 (3)
$In1^{i}$—La4—$Ru2^{xxv}$	103.89 (6)	La2i—Ru5—La2i	75.781 (11)
$In1^{xxv}$—La4—$Ru2^{xxv}$	0.00 (4)	La2i—Ru5—La2	74.64 (3)
$Ru2^{i}$—La4—$Ru2^{xxv}$	103.89 (6)	La2i—Ru5—La2	120.58 (2)
$Ru1^{xxiv}$—La4—La5	88.13 (4)	La2i—Ru5—La2	75.781 (11)
$Ru1^{iii}$—La4—La5	88.13 (4)	La2i—Ru5—La2	71.96 (3)
$Ru3^{xxv}$—La4—La5	148.90 (3)	La2i—Ru5—La2	139.13 (3)
$Ru3^{ii}$—La4—La5	148.90 (3)	La2i—Ru5—La2i	75.781 (11)
$In1^{i}$—La4—La5	51.94 (3)	La2i—Ru5—La2i	71.96 (3)
$In1^{xxv}$—La4—La5	51.94 (3)	La2i—Ru5—La2i	139.13 (3)
$Ru2^{i}$—La4—La5	51.94 (3)	La2i—Ru5—La2i	120.58 (2)
$Ru2^{xxv}$—La4—La5	51.94 (3)	La2i—Ru5—La2i	75.781 (11)
$Ru1^{xxiv}$—La4—$La3^{iii}$	134.76 (5)	La2—Ru5—La2i	143.22 (3)
$Ru1^{iii}$—La4—$La3^{iii}$	48.97 (3)	La2i—Ru5—La2i	71.96 (3)
$Ru3^{xxv}$—La4—$La3^{iii}$	51.15 (3)	La2i—Ru5—La2i	75.781 (11)
$Ru3^{ii}$—La4—$La3^{iii}$	51.15 (3)	La2i—Ru5—La2i	120.58 (2)
$In1^{i}$—La4—$La3^{iii}$	116.846 (17)	La2i—Ru5—La2i	139.13 (3)
$In1^{xxv}$—La4—$La3^{iii}$	116.845 (17)	La2i—Ru5—La2i	143.22 (3)
$Ru2^{i}$—La4—$La3^{iii}$	116.846 (17)	La2—Ru5—La2i	75.781 (11)
$Ru2^{xxv}$—La4—$La3^{iii}$	116.845 (17)	La2i—Ru5—La2i	74.64 (3)
La5—La4—$La3^{iii}$	137.10 (2)	La1—In2—La1i	180.00 (3)
$Ru1^{xxiv}$—La4—$La3^{xvii}$	48.97 (3)	La1—In2—La1i	70.717 (10)
$Ru1^{iii}$—La4—$La3^{xvii}$	134.76 (5)	La1i—In2—La1i	109.283 (10)
$Ru3^{xxv}$—La4—$La3^{xvii}$	51.15 (3)	La1—In2—La1i	109.85 (2)
$Ru3^{ii}$—La4—$La3^{xvii}$	51.15 (3)	La1i—In2—La1i	70.15 (2)
$In1^{i}$—La4—$La3^{xvii}$	116.845 (17)	La1i—In2—La1i	70.717 (10)
$In1^{xxv}$—La4—$La3^{xvii}$	116.845 (17)	La1—In2—La1i	70.717 (10)
$Ru2^{i}$—La4—$La3^{xvii}$	116.845 (17)	La1i—In2—La1i	109.283 (10)
$Ru2^{xxv}$—La4—$La3^{xvii}$	116.845 (17)	La1i—In2—La1i	109.85 (2)
La5—La4—$La3^{xvii}$	137.10 (2)	La1i—In2—La1i	70.717 (10)
$La3^{iii}$—La4—$La3^{xvii}$	85.79 (4)	La1—In2—La1i	109.283 (10)
$Ru1^{xxiv}$—La4—La1	119.600 (14)	La1i—In2—La1i	70.717 (10)
$Ru1^{iii}$—La4—La1	61.370 (13)	La1i—In2—La1i	70.15 (2)
$Ru3^{xxv}$—La4—La1	103.96 (4)	La1i—In2—La1i	109.283 (10)
$Ru3^{ii}$—La4—La1	50.94 (3)	La1i—In2—La1i	180.00 (3)
$In1^{i}$—La4—La1	58.39 (2)	La1—In2—La1i	70.15 (2)

In1^{xxv}—La4—La1	143.53 (3)	La1i—In2—La1i	109.85 (2)
Ru2^{i}—La4—La1	58.39 (2)	La1i—In2—La1i	109.283 (10)
Ru2^{xxv}—La4—La1	143.53 (3)	La1i—In2—La1i	180.00 (2)
La5—La4—La1	103.13 (2)	La1i—In2—La1i	109.283 (10)
La3^{iii}—La4—La1	60.151 (15)	La1i—In2—La1i	70.717 (10)
La3^{xvii}—La4—La1	99.50 (3)	La1—In2—La1i	109.283 (10)
Ru1^{xxiv}—La4—La1^{v}	61.370 (13)	La1i—In2—La1i	70.717 (10)
Ru1^{iii}—La4—La1^{v}	119.600 (14)	La1i—In2—La1i	180.00 (2)
Ru3^{xxv}—La4—La1^{v}	103.96 (4)	La1i—In2—La1i	109.283 (10)
Ru3^{ii}—La4—La1^{v}	50.94 (3)	La1i—In2—La1i	70.15 (2)
In1^{i}—La4—La1^{v}	58.39 (2)	La1i—In2—La1i	109.85 (2)
In1^{xxv}—La4—La1^{v}	143.53 (3)	La1i—In2—La1i	70.717 (10)
Ru2^{i}—La4—La1^{v}	58.39 (2)		

Symmetry codes: (i) $x-1/2, -y+1/2, z$; (ii) $x-1/2, -y+1/2, -z$; (iii) $x-1, y, z$; (iv) $-y, x, z$; (v) $-y+1/2, -x+1/2, z$; (vi) $x, y, -z$; (vii) $y, -x, z$; (viii) $-x+1, -y, z$; (ix) $x, -y, -z+1/2$; (x) $y, x, -z+1/2$; (xi) $-x+1, y, -z+1/2$; (xii) $-x+1/2, -y+1/2, -z+1/2$; (xiii) $-x+1/2, y-1/2, z$; (xiv) $x+1/2, -y+1/2, -z$; (xv) $-x+3/2, y+1/2, z$; (xvi) $x+1, y, z$; (xvii) $-x+1, -y+1, -z$; (xviii) $y+1/2, x+1/2, -z$; (xix) $x+1, y, -z$; (xx) $y+1/2, x+1/2, z$; (xxi) $-y+1, x, -z$; (xxii) $x+1/2, -y+1/2, z$; (xxiii) $-y+1, x, z$; (xxiv) $-x+1, -y+1, z$; (xxv) $-x+1/2, y+1/2, z$; (xxvi) $y-1/2, x+1/2, z$; (xxvii) $-x, -y+1, z$; (xxviii) $y, -x+1, z$; (xxix) $x-1/2, y+1/2, -z+1/2$; (xxx) $x, -y+1, -z+1/2$; (xxxi) $-y, -x+1, -z+1/2$; (xxxii) $y+1/2, -x+1/2, -z+1/2$; (xxxiii) $-x+3/2, y-1/2, z$; (xxxiv) $-x, -y, z$; (xxxv) $-y, -x, -z+1/2$; (xxxvi) $-x, y, -z+1/2$; (xxxvii) $-x, -y, -z$; (xxxviii) $-y, x, -z$; (xxxix) $y, -x, -z$.

Fig. 1


a
b
c
La1i
Ru3v
La3iii
La4iv
Ru1iii
Ru4vi
La2ii
La5iv
Ru5vi
In1vii
In2vii
La
Ru
InRu
In